

## Supplementary Material

### DS\*: Tighter Lifting-Free Convex Relaxations for Quadratic Matching Problems

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#### 1. Proofs

**Proposition 3.** *If a minimiser  $\tilde{x}$  of a faithful convex underapproximation  $F_{\text{conv}}$  of  $G + \delta_C$  meets  $\tilde{x} \in C$ , it is also a global minimiser of  $G + \delta_C$ .*

*Proof.* Assume that our statement is false. Then there exists a  $x \in C$  with  $G(x) < G(\tilde{x})$ . However, since  $F_{\text{conv}}$  is faithful, we have  $G(\tilde{x}) = F_{\text{conv}}(\tilde{x})$  as well as  $G(x) = F_{\text{conv}}(x)$ . We conclude  $F_{\text{conv}}(x) < F_{\text{conv}}(\tilde{x})$  which contradicts  $\tilde{x}$  being a minimiser of  $F_{\text{conv}}$ . ■

**Proposition 4.** *If  $F_{\text{conv}}^1$  and  $F_{\text{conv}}^2$  are two convex underapproximations of  $G + \delta_C$ , where  $F_{\text{conv}}^1$  is faithful and  $F_{\text{conv}}^2$  is not, then  $F_{\text{conv}}^2$  cannot be tighter than  $F_{\text{conv}}^1$ .*

*Proof.* Since  $F_{\text{conv}}^2$  is not faithful, there exists a  $x \in C$  for which  $F_{\text{conv}}^2(x) \neq G(x)$ . Because  $F_{\text{conv}}^2$  is still an underapproximation of  $G + \delta_C$ , it must hold that  $F_{\text{conv}}^2(x) < G(x) = F_{\text{conv}}^1(x)$ , which shows that  $F_{\text{conv}}^2$  cannot be tighter than  $F_{\text{conv}}^1$ . ■

**Proposition 5.** *Let  $X \in \mathbb{P}_n$  and  $x = \text{vec}(X)$ . For any  $d \in \mathbb{R}^{n^2}$ ,  $D_1, D_2 \in \mathbb{R}^{n \times n}$  it holds that  $f(x) = \tilde{f}(x; D_1, D_2, d)$ .*

*Proof.* With  $X \in \mathbb{P}_n$ , we have  $X^T X = \mathbf{I}_n$  and therefore

$$\langle \mathbf{I}_n, D_1 \rangle = \langle X^T X, D_1 \rangle, \quad (1)$$

$$= \langle X D_1, X \rangle = \langle \text{vec}(X D_1), \text{vec}(X) \rangle, \quad (2)$$

$$= \langle (D_1^T \otimes \mathbf{I}_n)x, x \rangle, \quad (3)$$

$$= x^T (D_1 \otimes \mathbf{I}_n)x. \quad (4)$$

Similarly  $\langle \mathbf{I}_n, D_2 \rangle = x^T (\mathbf{I}_n \otimes D_2)x$ . Moreover, since  $X \in \mathbb{P}_n$ , we have that  $X_{ij} = X_{ij}^2$  for all  $i, j = 1, \dots, n$ . Thus,  $x^T \text{diag}(d)x = d^T x$ . Combining the above shows that  $f(x) - \tilde{f}(x; D_1, D_2, d) = x^T (D_1 \otimes \mathbf{I}_n + \mathbf{I}_n \otimes D_2 + \text{diag}(d))x - d^T x - \langle \mathbf{I}_n, D_1 + D_2 \rangle = 0$ . ■

**Lemma 6.** *Let  $D, D' \in \mathbb{R}^{n \times n}$  be symmetric and let  $d, d' \in \mathbb{R}^{n^2}$ . Define  $\hat{D} = D' - D$ . If  $d_i \leq d'_i$  for all  $i = 1, \dots, n^2$ ,*

*as well as  $\hat{D}_{ii} - \max_{j \neq i}(\max(\hat{D}_{ij}, 0)) \geq 0$  for all  $i = 1, \dots, n$ , then it holds for all  $x \in \text{vec}(\mathbb{DS}_n)$*

$$\tilde{f}(x; D, \bullet, \circ) \leq \tilde{f}(x; D', \bullet, \circ), \quad (5)$$

$$\tilde{f}(x; \diamond, D, \circ) \leq \tilde{f}(x; \diamond, D', \circ), \text{ and} \quad (6)$$

$$\tilde{f}(x; \diamond, \bullet, d) \leq \tilde{f}(x; \diamond, \bullet, d'), \quad (7)$$

where  $\diamond \in \mathbb{R}^{n \times n}$ ,  $\bullet \in \mathbb{R}^{n \times n}$  and  $\circ \in \mathbb{R}^{n^2}$ .

*Proof.* We have

$$\tilde{f}(x; D, \bullet, \circ) - \tilde{f}(x; D', \bullet, \circ) \quad (8)$$

$$= x^T (-Z(D, \bullet, \circ) + Z(D', \bullet, \circ))x - \langle \mathbf{I}_n, \hat{D} \rangle \quad (9)$$

$$= x^T (D' \otimes \mathbf{I}_n - D \otimes \mathbf{I}_n)x - \langle \mathbf{I}_n, \hat{D} \rangle \quad (10)$$

$$= x^T ((D' - D) \otimes \mathbf{I}_n)x - \langle \mathbf{I}_n, \hat{D} \rangle \quad (11)$$

$$= \langle X^T X, \hat{D} \rangle - \langle \mathbf{I}_n, \hat{D} \rangle \quad (12)$$

$$= \sum_i \left( (X^T X)_{ii} - 1 \right) \hat{D}_{ii} + \sum_{j \neq i} (X^T X)_{ij} \hat{D}_{ij}. \quad (13)$$

We continue by looking at (13) for each  $i$  separately:

$$((X^T X)_{ii} - 1) \hat{D}_{ii} + \sum_{j \neq i} (X^T X)_{ij} \hat{D}_{ij} \quad (14)$$

$$\leq ((X^T X)_{ii} - 1) \hat{D}_{ii} + \sum_{j \neq i} (X^T X)_{ij} \max(\hat{D}_{ij}, 0) \quad (15)$$

$$\leq (1 - (X^T X)_{ii}) (-\hat{D}_{ii}) + \left( \max_{j \neq i}(\max(\hat{D}_{ij}, 0)) \right) \sum_{j \neq i} (X^T X)_{ij} \quad (16)$$

$$= \underbrace{(1 - (X^T X)_{ii})}_{\geq 0} \underbrace{\left( \max_{j \neq i}(\max(\hat{D}_{ij}, 0)) - \hat{D}_{ii} \right)}_{\leq 0 \text{ by assumption}} \quad (17)$$

$$\leq 0. \quad (18)$$

In the step from (16) to (17) we used that if  $X$  is doubly-stochastic, then so is  $X^T X$ . Thus, using (13) it follows that

$\tilde{f}(x; D, \bullet, \circ) \leq \tilde{f}(x; D', \bullet, \circ)$ . The case in (6) is analogous. Note that tighter (but more complicated criteria) can be derived by additionally considering the sum over  $i$  and using that  $(X^T X)_{i,i} \geq \frac{1}{n}$ . We skipped this analysis for the sake of simplicity.

Moreover,

$$\tilde{f}(x; \diamond, \bullet, d) - \tilde{f}(x; \diamond, \bullet, d') \quad (19)$$

$$= x^T (-Z(\diamond, \bullet, d) + Z(\diamond, \bullet, d'))x + (d - d')^T x \quad (20)$$

$$= x^T (\text{diag}(d') - \text{diag}(d))x + (d - d')^T x \quad (21)$$

$$= x^T (\text{diag}(d' - d))x + (d - d')^T x \quad (22)$$

$$= \sum_{i=1}^{n^2} (d' - d)_i x_i^2 + (d - d')_i x_i \quad (23)$$

$$= \sum_{i=1}^{n^2} (d' - d)_i x_i^2 - (d' - d)_i x_i \quad (24)$$

$$= \sum_{i=1}^{n^2} (d' - d)_i (x_i^2 - x_i) \leq 0. \quad (25)$$

The last inequality follows from the assumption  $d'_i - d_i \geq 0$  and  $x_i^2 - x_i \leq 0$  (using  $x \in \text{vec}(\mathbb{DS}_n)$ ). ■

**Proposition 7.** *The minimiser  $\tilde{\Delta}$  among all  $\Delta = (D_1, D_2, d)$  with symmetric  $D_1$  and  $D_2$  of*

$$\min_{\Delta} -\text{tr}(Z(\Delta)) + \frac{1}{n} \sum_{i,j} (Z(\Delta))_{ij} \quad (26)$$

$$\begin{aligned} \text{s.t.} \quad & F^T(W - Z(\Delta))F \succeq 0, \\ & 0 \geq -(D_1)_{ii} + \max_{j \neq i} \max((D_1)_{ij}, 0) \quad \forall i, \\ & 0 \geq -(D_2)_{ii} + \max_{j \neq i} \max((D_2)_{ij}, 0) \quad \forall i, \\ & d_i \geq \lambda_{\min}^* \quad \forall i, \end{aligned}$$

yields a relaxation that is at least as tight as DS++. If  $Z(\tilde{\Delta}) \neq \lambda_{\min}^* \mathbf{I}_{n^2}$ , the above is tighter than DS++.

*Proof.* First of all, we observe that, in addition to  $\Delta_{\text{DS++}} = (\lambda_{\min}^* \mathbf{I}_n, \mathbf{0}, \mathbf{0})$ , the DS++ relaxation is also obtained by the choice  $\Delta'_{\text{DS++}} = (\mathbf{0}, \mathbf{0}, \lambda_{\min}^* \mathbf{1}_{n^2})$ . The constraints in (26) are feasible as they are satisfied for the DS++ choice  $\Delta'_{\text{DS++}} = (\mathbf{0}, \mathbf{0}, \lambda_{\min}^* \mathbf{1}_{n^2})$ . Thus, a minimiser exists.

Writing  $\tilde{\Delta} = (\tilde{D}_1, \tilde{D}_2, \tilde{d})$ , the convex constraints immediately yield that

$$\begin{aligned} \tilde{f}(x; \lambda_{\min}^* \mathbf{I}_n, \mathbf{0}, \mathbf{0}) &= \tilde{f}(x; \mathbf{0}, \mathbf{0}, \lambda_{\min}^* \mathbf{1}_{n^2}) \\ &\leq \tilde{f}(x; \mathbf{0}, \mathbf{0}, \tilde{d}) \\ &\leq \tilde{f}(x; \tilde{D}_1, \mathbf{0}, \tilde{d}) \\ &\leq \tilde{f}(x; \tilde{D}_1, \tilde{D}_2, \tilde{d}) = f(x; \tilde{\Delta}) \end{aligned}$$

holds for all  $x \in \text{vec}(\mathbb{DS}_n)$  based on Lemma 6.

Finally, one can compare  $\tilde{f}(x; \tilde{\Delta})$  with  $\tilde{f}(x; \Delta'_{\text{DS++}})$  at  $x = \frac{1}{n} \mathbf{1}_{n^2}$  to see that the DS++ relaxation is strictly below the relaxation given by (26) if DS++ does not happen to yield a solution to (26) already. ■

**Lemma 8.** *Let  $T(d_1, d_2)$  have a smallest eigenvalue  $\lambda_{\min}$  of multiplicity 1, and let  $u_{\min}$  be a corresponding eigenvector with  $\|u_{\min}\| = 1$ . Then*

$$(p_1)_j = -\min(\lambda_{\min}, 0) \sum_i ((\text{vec}^{-1}(F u_{\min}))_{i,j})^2,$$

$$(p_2)_i = -\min(\lambda_{\min}, 0) \sum_j ((\text{vec}^{-1}(F u_{\min}))_{i,j})^2$$

meet  $p_1 = \nabla_{d_1}(h \circ T)(d_1, d_2)$ ,  $p_2 = \nabla_{d_2}(h \circ T)(d_1, d_2)$ .

*Proof.* The proof is based on the fact that  $(h \circ T)$  is a composition of four functions:

$$(h \circ T)(d_1, d_2) = \frac{1}{2} \min(g(\lambda(T(d_1, d_2))), 0)^2,$$

i.e. the affine function  $T$ , a function  $Y \mapsto \lambda(Y)$  determining the eigenvalues of  $Y$ , a function  $g(v) = \min(v)$  selecting the minimal element of a vector, and the function  $x \mapsto \frac{1}{2} \min(x, 0)^2$ . The latter is continuously differentiable with derivative  $\min(x, 0)$ .

Compositions of the form  $g(\lambda(Y))$  have been studied in detail in [2], and according to [2, p. 585, Example of Cox and Overton] it holds that

$$\partial(g \circ \lambda)(Y) = \text{conv}\{uu^T : Yu = \lambda_{\min}(Y)u, \|u\| = 1\}. \quad (27)$$

Note that  $(g \circ \lambda)$  becomes differentiable if the smallest eigenvalue of  $Y$  has multiplicity one, such that the corresponding eigenspace is of dimension 1 and the above set  $\partial(g \circ \lambda)(Y)$  reduces to a singleton – also see [2, Theorem 2.1].

Thus, by the chain rule

$$\min(\lambda_{\min}(Y), 0) u_{\min} u_{\min}^T$$

is a gradient of  $h$  at  $Y$  if  $\lambda_{\min}(Y)$  has multiplicity 1.

Left to consider is the inner derivative coming from the affine map  $T$ . Let us consider the linear operator

$$\tilde{T}(d_1) = -F^T(\text{diag}(d_1) \otimes \mathbf{I}_n)F$$

as the part of  $T$  that has a relevant inner derivative with respect to  $d_1$ . The gradient of a linear operator  $\tilde{T}$  is nothing but its adjoint operator  $\tilde{T}^*$ , i.e. the operator for which

$$\langle \tilde{T}(d), A \rangle = \langle d, \tilde{T}^*(A) \rangle$$

holds for all  $d$  and all  $A$ . (In this case we could explicitly prove this by vectorizing the entire problem, but the relation holds in much more generality as the definition of general

(Gateaux) gradients utilises the Riesz representation theorem, see e.g. [1, p. 40, Remark 2.55]). Since the adjoint of  $T_1 \circ T_2$  is  $T_2^* \circ T_1^*$ , we can consider the operations separately in a reverse order. The last thing  $\tilde{T}$  does is the multiplication with  $F^T$  from the left and with  $F$  from the right, which means that the first thing the adjoint  $\tilde{T}^*$  does is the multiplication with  $F$  from the left and with  $F^T$  from the right.

The operator  $\text{diag}(d_1) \otimes \mathbf{I}_n$  repeats the entries of  $d_1$   $n$  times, and writes the result on the diagonal of an  $n^2 \times n^2$  diagonal matrix. The adjoint of writing a vector of length  $n^2$  on the diagonal of an  $n^2 \times n^2$  diagonal matrix, is the extraction of the diagonal of such a matrix. Finally, the adjoint of the repeat operation is the summation over the components of those indices at which values were repeated. As an illustrative example, note that

$$\underbrace{A = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}}_{\text{repeat each component}} \Rightarrow A^* = \underbrace{\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}}_{\text{sum over repeated components}}.$$

If  $\tilde{T}^*$  is applied to an element  $Y = uu^T \in \mathbb{R}^{n^2 \times n^2}$  the first steps are left multiplication with  $F$  and right multiplication with  $F^T$ , leading to  $(Fu)(Fu)^T$ . The extraction of the diagonal of the resulting matrix yields a vector of length  $n^2$  with entries  $(Fu)_k^2$ . By taking sums over  $n$  consecutive entries, and multiplying with the remaining inner derivatives  $(-1)$  and  $\min(\lambda_{\min}, 0)$  we arrive at the formula for  $\nabla_{d_1}(h \circ T)$  as stated by Lemma 8. Determining the formula for  $\nabla_{d_2}(h \circ T)$  follows exactly the same computation with a different final summation as the operator  $\mathbf{I}_n \otimes \text{diag}(d_2)$  repeats the entries in a different order. ■

**Lemma 9.** Let  $x^i \in \mathbb{R}^n$  be defined as

$$(x^i)_j := \begin{cases} 1 & \text{if } j = i \\ -1 & \text{if } j = i + 1, \\ 0 & \text{otherwise} \end{cases}, \quad \text{and let } z^{i,j} := x^i \otimes x^j.$$

With  $F = [z^{1,1}, z^{1,2}, \dots, z^{n-1,n-1}] \in \mathbb{R}^{n^2 \times (n-1)^2}$ , we have that  $\text{im}(F) = \ker(A)$  for  $A = \begin{bmatrix} \mathbf{I}_n \otimes \mathbf{1}_n^T \\ \mathbf{1}_n^T \otimes \mathbf{I}_n \end{bmatrix}$ .

*Proof.* The linear independence of all  $x^1, \dots, x^{n-1}$  implies the linear independence of all  $z^{i,j} = x^i \otimes x^j$  for  $i, j \in [n-1]$ , from which we see that  $\dim(\text{im}(F)) = \text{rank}(F) = (n-1)^2 = n^2 - 2n + 1 = \dim(\ker(A))$ .

We proceed by showing that  $\text{im}(F) \subseteq \ker(A)$ . Let  $z \in \text{im}(F)$ , so  $z = \sum_{i,j=1}^{n-1} a_{ij} z^{i,j}$  for some coefficients  $\{a_{ij} \in \mathbb{R}\}$ . By construction of the  $z^{i,j}$ , for  $i, j \in [n-1]$  we have

$$(\mathbf{I}_n \otimes \mathbf{1}_n^T) z^{i,j} = \mathbf{0}_n \quad \text{and} \quad (\mathbf{1}_n^T \otimes \mathbf{I}_n) z^{i,j} = \mathbf{0}_n, \quad (28)$$

which implies that

$$(\mathbf{I}_n \otimes \mathbf{1}_n^T) a_{ij} z^{i,j} = \mathbf{0}_n \quad \text{and} \quad (\mathbf{1}_n^T \otimes \mathbf{I}_n) a_{ij} z^{i,j} = \mathbf{0}_n. \quad (29)$$

Thus

$$(\mathbf{I}_n \otimes \mathbf{1}_n^T) z = \mathbf{0}_n \quad \text{and} \quad (\mathbf{1}_n^T \otimes \mathbf{I}_n) z = \mathbf{0}_n, \quad (30)$$

from which we can see that  $z \in \ker(A)$ . Combining  $\dim(\text{im}(F)) = \dim(\ker(A))$  and  $\text{im}(F) \subseteq \ker(A)$  shows that  $\text{im}(F) = \ker(A)$ . ■

## References

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- [2] A. S. Lewis. Derivatives of spectral functions. *Mathematics of Operations Research*, 1996. 2